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Composition of the essential oil of *Caucalis platycarpos* L.*

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Results of the investigation of the composition of the essential oil obtained by hydrodistillation of the aerial parts of *Caucalis platycarpos* L. (*Apiaceae*) are presented. Essential oil was analyzed by GC-MS. The oil proved to be rich in sesquiterpenes. Spathulenol (10.0%) was the main compound of the oil.

Keywords: Caucalis platycarpos L. (*Apiaceae*), essential oil, GC-MS

Caucalis platycarpos L. (= *Caucalis daucoides* L., *Caucalis lappula* Grande) is an annual herb, belonging to the family *Apiaceae*, of widespread distribution in the Mediterranean and Central Europe. It is up to 40 cm high, with leaves pinnately divided into oblong or lanceolate lobes, almost glabrous, white or pink flowers, and ellipsoid to ovoid fruits (1).

The dried decoction of this plant showed a remarkable antitumor activity as a consequence of the stimulation of the immunological system of the host (2).

Chemical investigations have detected a number of constituents, including flavonoids, essential oil, starch, cellulose, proteins, carbohydrates, lignin, tannins, β-sitosterol and scopoletin (3–5).

This work represents the first detailed investigation of the composition of the essential oil of the aerial parts of *Caucalis platycarpos* L.

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EXPERIMENTAL

Plant material

Aerial parts of *C. platycarpos* were collected in 1998 in the surroundings of Imotski (Croatia). Voucher specimen (No. 99100) has been deposited in the Herbarium of the Department of Pharmacognosy, Faculty of Pharmacy and Biochemistry (University of Zagreb, Croatia). Moisture content was determined on the basis of the loss by drying according to the method of ÖAB (11).

Distillation of the essential oil

The sample was air dried in the shadow and cut into small pieces before distilling. Hydrodistillation of the essential oil was carried out for 2 h in an apparatus according to Eur. Ph. (6).

GC-MS analysis

The analysis was performed on a HP 5890 Series II Plus gas chromatograph interfaced to a HP 5989B mass spectrometer (Hewlett-Packard, USA); columns: 1. fused silica capillary column Ultra 2 (Hewlett-Packard) (l = 46 m, ID = 0.20 mm) with 5%Phe95%Me silicone as stationary phase, coating thickness 0.11 μm; 2. fused silica capillary column DB Wax (J&W Scientific) (l = 57 m, ID = 0.25 mm), stationary phase polyethylene glycol, coating thickness 0.25 μm.

Working conditions for Ultra 2 column: injector temperature 250 °C, interface temperature 280 °C; linear oven temperature program from 70–200 °C with 2 °C min^{-1}, carrier gas: helium 5.0, flow rate: 1.0 mL min^{-1}, split ratio 40:1. Working conditions for DB Wax column: injector temperature 230 °C, interface temperature 250 °C, linear oven temperature program from 70–230 °C with 2 °C min^{-1}, carrier gas: helium 5.0, flow rate: 1.0 mL min^{-1}, split ratio 40:1.

The mass spectrometer operated in the electron ionization mode (70 eV), ion source temperature was 200 °C, quadrupol temperature was 100 °C.

The compounds were identified upon comparison with reference compounds, mass spectra library search and retention index references (7–10).

Quantification of the relative amounts of individual components was done according to the area percent method, disregarding calibration factors.

RESULTS AND DISCUSSION

Hydrodistillation of the aerial parts of *C. platycarpos* yielded 0.05% (V/m) of essential oil (calculated on the dry mass basis, taking a moisture content of the dried plant material of 5.6% into account).

The essential oil was analyzed by GC-MS using two stationary phases of different polarity. The results are shown in Table I. The composition of the oil was rather complex.

Table I. Composition (%) of the essential oil of Caucalis platycarpos *L.*

No.	Compound	Area (%)	RI (polar) (DB-Wax)	Identification[a]
1	α-Pinene	0.3	1030	1,2,3
2	(E)-1,3-Nonadiene	0.9	1052	2
3	Camphene	<0.1	1076	1,2,3
4	β-Pinene	<0.1	1119	1,2,3
5	Sabinene	0.2	1127	1,2,3
6	α-Terpinene	0.3	1186	1,2,3
7	Limonene	0.1	1206	1,2,3
8	β-Phellandrene	0.1	1215	2
9	2-Pentylfurane	0.1	1230	2
10	γ-Terpinene	0.8	1248	1,2,3
11	*p*-Cymene	0.4	1272	1,2,3
12	α-Terpinolene	0.4	1287	1,2,3
13	1-Octanal	0.2	1289	1,2,3
14	1-Nonanal	0.8	1392	1,2,3
15	*p*-Mentha-1,5,8-triene	0.2	1427	2
16	1-Methyl-2-(2-propenyl)-benzene	0.3	1434	2
17	Linalooloxide (*trans*)	0.5	1441	2,3
18	α-Cubenene	0.1	1458	1,2,3
19	Linalooloxide (*cis*)	0.2	1469	2,3
20	2-Ethyl-1-hexanol	0.3	1486	2
21	α-Campholenaldehyde	0.1	1491	2
22	α-Copaene	0.1	1493	1,2,3
23	Dihydroedulan II	0.4	1494	2,3
24	3-Nonen-2-one	0.4	1508	2
25	(E)-2-Nonenal	3.8	1531	2
26	Linalool	1.6	1542	1,2,3
27	1-Octanol	0.5	1554	2,3
28	β-Elemene	0.2	1587	2,3
29	*trans*-Caryophyllene	1.0	1596	1,2,3
30	Terpinen-4-ol	2.2	1600	1,2,3
31	*p*-1-Menthen-9-al	1.7/1.5	1611/1615	2
32	γ-Elemene	0.3	1636	2,3
33	2,6,6-Trimethyl-1,3-cyclohexadiene-1-carboxaldehyde	0.3	1641	2
34	1-Nonanol	0.5	1658	2
35	α-Terpineol	1.0	1694	1,2,3
36	α-Muurolene	0.8	1722	2,3
37	δ-Cadinene	1.7	1755	2,3
38	1-Decanol	0.2	1761	2
39	4-(1-Methylethyl)-benzaldehyde	0.3	1774	2
40	β-Damascenone	0.5	1817	2,3
41	(1E, 4Z)-Germacrene B	1.3	1826	2,3
42	*trans*-Geraniol	0.6	1845	2,3
43	6,10-Dimethyl-5,9-undecadien-2-one	0.6	1850	2
44	β-Jonone	1.2	1934	2
45	Caryophyllenoxide	3.1	1979	2,3
46	Spathulenol	10.0	2120	2,3
47	6,10,14-Trimethyl-2-pentadecanone	0.8	2143	2
48	T-Muurolol	0.8	2183	2
49	2-Hydroxy-5-methoxybenzaldehyde	2.0	2405	2

[a] Mode of identification: 1 – co-GC (with reference compounds); 2 – MS-library search (Wiley 138K and own laboratory data base); 3 – comparison of retention indices with refs. 7–10

Forty-nine compounds, representing about 45% of the total peak area could be identified, while a number of peaks with M_r = 220 and 222 could only be classified as oxidized sequiterpenes. Altogether, 12 monoterpene hydrocarbons were identified, γ-terpinene (0.8%) being the main compound in this group. Sesquiterpene hydrocarbons were present in minor amounts as well. Major representatives of this class of compounds (of 8 identified) were δ-cadinene (1.7%), (1E, 4Z)-germacrene B (1.3%), and *trans*-caryophyllene (1.0%). Oxidized monoterpenes and sesquiterpenes were present in higher percentages. Nine oxidized monoterpenes could be found in the essential oil; terpinen-4-ol (2.2%) and linalool (1.6%) were the major compounds in this fraction. Two adjacent peaks with linear retention indices of 1611/1615 (polar column) and 1214/1216 (non polar column) showed identical mass spectra of *p*-1-menthen-9-al; two stereoisomers are most probably present in the oil. *p*-1-Menthen-9-al was previously found, among others, in some *Umbelliferae* oils (12, 13). Only a few reference spectra were available for oxidised sequiterpenes. Spathulenol represented the major compound of the oil (10.0%).

Noticable amounts of compounds belonging to classes other than mono- or sesquiterpenes were present, such as the aldehydes 1-octanal, 1-nonanal and (E)-2-nonenal (3.8%). Two benzaldehydes (4-(1-methylethyl))-benzaldehyde and 2-hydroxy-5-methoxybenzaldehyde) were identified as well. Dihydroedulan II (2,3,4,4a,5,6-hexahydro-2,5,5,8a-tetramethyl-(8aH)-1-benzopyrane), originally found as a trace compound in the juice of *Passiflora edulis* (10), was previously also identified in the essential oil obtained from another *Apiaceae* species, *Aegopodium podagraria* (8).

In an earlier investigation, Williams and Harborne (4) detected high amounts of β-pinene (9%) in the essential oil obtained from the fruits of *C. platycarpos*. Our analysis revealed β-pinene only as a trace compound in the oil of the aerial parts. Hence, further analyses dealing with the variation of the oil composition should be carried out.

CONCLUSIONS

The essential oil of the aerial parts of *Caucalis platycarpos* contained monoterpene and sesquiterpene hydrocarbons only in smaller amounts, whereas oxidized monoterpenes and sesquiterpenes were present in higher percentages. Furthermore, a number of compounds belonging to classes other than mono- and sesquiterpenes, namely aldehydes like (E)-2-nonenal, two benzaldehydes and dihydroedulan II, were identified.

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SAŽETAK

Istraživanje kemijskog sastava eteričnog ulja podlanice – *Caucalis platycarpos* L.

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Eterično ulje nadzemnih dijelova podlanice – *Caucalis platycarpos* L. (*Apiaceae*) dobiveno je postupkom hidrodestilacije, a njegov kemijski sastav analiziran je kombiniranom tehnikom plinske kromatografije i spektrometrije masa. Najzastupljenije sastavnice eteričnog ulja bili su seskviterpeni, posebice spatulenol (10,0%).

Ključne riječi: Caucalis platycarpos L. (*Apiaceae*), eterično ulje, plinska kromatografija-spektrometrija masa

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